Ising model (cont'd)

PHYS 250 (Autumn 2018) – Lecture 7

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Outline

Outline of the Ising model discussion

We've already discussed a lot, and I want to remind you of those topics, their progression, and where we're going from here to make sure that we're all on the same page.

- Lecture 5: the model iteself
  - The general concept of the model: lattice of spins
  - Basis in thermodynamics and quantum mechanics
  - Importance of simulations methods
- Lecture 6: computational approaches
  - History of computational simulation methods: Monte Carlo
  - The Metropolis Monte Carlo algorithm and its assumptions (deeply related to thermodynamics)
- Lecture 7 (Today): analytical and computational evaluation
  - Analytical Ising model and the key numerical results
  - Concept of equilibrium and how we can define it
  - Observables in the Ising model and their calculation
- "Lecture 8" (Tomorrow): Hands-on lab+lecture
  - Hands-on session in CSIL 2 for developing our Ising model simulation

Outline

Recall our discussion of statistical mechanics

We discussed that the probability distribution of an observable such as the mean energy, $\langle E \rangle$, of a system in a particular microstate μ is given by

$$\langle E \rangle = \frac{\sum_\mu E_\mu e^{-\beta E_\mu}}{\sum_\mu e^{-\beta E_\mu}} = \frac{\sum_\mu e^{-\beta E_\mu}}{Z} \tag{1}$$

where Z is the **partition function** of the system. Focusing just on the numerator for a moment, this can be recast in terms of Z:

$$\sum_\mu E_\mu e^{-\beta E_\mu} = -\sum_\mu \frac{\partial}{\partial \beta} \left(e^{-\beta E_\mu} \right) = -\frac{\partial Z}{\partial \beta} \tag{2}$$

We can then rewrite the mean energy in a much simpler form:

$$\langle E \rangle = -\frac{1}{Z} \frac{\partial Z}{\partial \beta} = -\frac{\partial \ln Z}{\partial \beta} \tag{3}$$

Similarly, the variance is given by:

$$Var(E) = \langle E^2 \rangle - \langle E \rangle^2 = -\frac{\partial \langle E \rangle}{\partial \beta} = \frac{\partial^2 \ln Z}{\partial \beta^2} \tag{4}$$

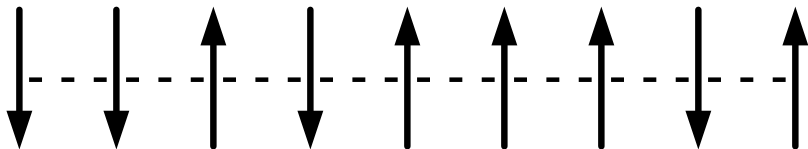## Ising's analytical solution for a 1D spin lattice

For a single dimension, and just $N = 2$ spins (the smallest possible Ising chain model) we can use the analytic form on the previous slide to write down Z exactly, and thus the mean energy (recall $E = -J \sum_{\langle ij \rangle} s_i s_j$) and its variance.

$$
\begin{aligned}
Z_2 &= \sum_{s_1 = \pm 1} \sum_{s_2 = \pm 1} e^{\beta J \sum_{i=1}^{N-1} s_i s_{i+1}} & (5) \\
&= e^{-\beta E(s_1 = +1, s_2 = +1)} + e^{-\beta E(s_1 = +1, s_2 = -1)} \\
&\quad + e^{-\beta E(s_1 = -1, s_2 = +1)} + e^{-\beta E(s_1 = -1, s_2 = -1)} & (6) \\
&= 2 e^{\beta J} + 2 e^{-\beta J} & (7) \\
&= 4 \cosh \beta J & (8)
\end{aligned}
$$

Ising's analytical solution for a 1D spin lattice

We can generalize this to N spins, either by induction based on one more manual sum with $N = 3$, or by direct proof (which I leave to you!)

$$
\begin{align}
Z_3 &= \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \sum_{s_3=\pm 1} e^{\beta J \sum_{i=1}^{N-1} s_i s_{i+1}} \tag{9} \\
&= \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} \sum_{s_3=\pm 1} e^{\beta J s_1 s_2 + \beta J s_2 s_3} \tag{10} \\
&= \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} e^{\beta J s_1 s_2} \left[e^{\beta J s_2} + e^{-\beta J s_2} \right] \tag{11} \\
&= 2 \cosh \beta J \sum_{s_1=\pm 1} \sum_{s_2=\pm 1} e^{\beta J s_1 s_2} \tag{12} \\
&= (2 \cosh \beta J) \, Z_2 \tag{13} \\
Z_N &= (2 \cosh \beta J) \, Z_{N-1} \tag{14} \\
&= 2 \, (2 \cosh \beta J)^{N-1} \tag{15}
\end{align}
$$

Outline

Equilibrium

So what do we do with our Monte Carlo program for the Ising model, once we have written it? we probably want to know the answer to some questions like ?What is the magnetization at such-and-such a temperature??, or ?How does the internal energy behave with temperature over such-and- such a range?? To answer these questions we have to do two things. First we have to run our simulation for a suitably long period of time until it has come to equilibrium at the temperature we are interested in. This period is called the equilibration time τ_{eq}. Then we have to measure the quantity we are interested in over another suitably long period of time and average it, to evaluate the estimator of that quantity. What exactly do we mean by ?allowing the system to come to equilibrium?? And how long is a ?suitably long? time for it to happen? How do we go about measuring our quantity of interest, and how long do we have to average over to get a result of a desired degree of accuracy? These are very general questions which we need to consider every time we do a Monte Carlo calculation.

?equilibrium? means that the average probability of finding our system in any particular state ? is proportional to the Boltzmann weight $e^{-\beta E_\mu}$ of that state. If we start our system off in a state such as the $T = 0$ (all spins aligned), and

Outline